NEWS IPC8

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For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 15:50:32 ON 07 JUN 2007

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

COST IN U.S. DOLLARS

FILE 'REGISTRY' ENTERED AT 15:51:34 ON 07 JUN 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4 DICTIONARY FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\161.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full FULL SEARCH INITIATED 15:52:17 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS SEARCH TIME: 00.00.01

0 ANSWERS

=> s l1 full

FULL SEARCH INITIATED 15:53:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED

20 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L3

0 SEA SSS FUL L1

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL SESSION

346.00

346.42

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 15:55:27 ON 07 JUN 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4 DICTIONARY FILE UPDATES: 6 JUN 2007 HIGHEST RN 936692-95-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\Stnexp\Queries\161a.str

L4 STRUCTURE UPLOADED

=> d ;4

L4 HAS NO ANSWERS

L4 STR

Structure attributes must be viewed using STN Express query preparation.

4 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 14 sss full

FULL SEARCH INITIATED 15:56:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED

29 ITERATIONS

27 ANSWERS

SEARCH TIME: 00.00.01

L5

27 SEA SSS FUL L4

=> d 15 1-27

L5 ANSWER 1 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 892396-78-0 REGISTRY

ED Entered STN: 13 Jul 2006

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (α S)- α -ethyl-2-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . C13 H15 N

SR CA

LC STN Files: CA, CAPLUS

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 254437-90-6 CMF C13 H15 N

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 892396-76-8 REGISTRY

ED Entered STN: 13 Jul 2006

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (αR) - α -ethyl-1-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . C13 H15 N

SR CA

LC STN Files: CA, CAPLUS

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 22038-83-1 CMF C13 H15 N

Absolute stereochemistry.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 3 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 892396-73-5 REGISTRY
- ED Entered STN: 13 Jul 2006
- CN Cinchonan-9-ol, $(8\alpha, 9R)$ -, mono[(-)- α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoate] (salt) (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 O7 S2 . C19 H22 N2 O
- SR CA
- LC STN Files: CA, CAPLUS

CM 1

CRN 549494-39-5

Absolute stereochemistry. Rotation (-).

CM 2

CRN 485-71-2 CMF C19 H22 N2 O

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 891182-81-3 REGISTRY

ED Entered STN: 10 Jul 2006

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . C4 H11 N

SR CA

LC STN Files: CA, CAPLUS, CASREACT

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CRN 75-64-9 CMF C4 H11 N

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 5 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 891182-74-4 REGISTRY

ED Entered STN: 10 Jul 2006

CN Benzenepropanoic acid, $4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-\alpha-[(2-phenylethyl)thio]-, (<math>\alpha$ S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O6 S2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 6 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 840494-28-2 REGISTRY
- ED Entered STN: 02 Mar 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, ion(1-) (9CI) (CA INDEX NAME)
- MF C26 H27 O7 S2
- CI COM
- SR CA

$$\begin{array}{c|c} O & CO_2 \\ \hline \\ O & CH_2 - CH_2 \\ \hline \end{array}$$

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L5 ANSWER 7 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
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RN 817642-79-8 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-[4-(1,1-dimethylethoxy)phenyl]ethyl]thi o]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2-[[2-(4-tert-Butoxyphenyl)ethyl]sulfanyl]-3-[4-[2-[4-[(methanesulfonyl)oxy]phenoxy]ethyl]phenyl]propionic acid

MF C30 H36 O7 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-S-O} \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH-S-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

∠ OBu-t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 8 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817642-78-7 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]-2-(phenylmethyl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3-[4-[2-[2-benzyl-4-[(methanesulfonyl)oxy]phenoxy]ethyl]phenyl]-2-[[2-(4-hydroxyphenyl)ethyl]sulfanyl]propionic acid

MF C33 H34 07 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 9 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 817642-76-5 REGISTRY
- ED Entered STN: 21 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfonyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-[[2-(4-Hydroxyphenyl)ethyl]sulfonyl]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C26 H28 O9 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

PAGE 1-B

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 10 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN:
- RN 817642-73-2 REGISTRY
- ED Entered STN: 21 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfinyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:
- CN 2-[[2-(4-Hydroxyphenyl)ethyl]sulfinyl]-3-[4-[2-[4-

[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C26 H28 O8 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

PAGE 1-B

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 11 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817642-72-1 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-(3-methoxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-[[2-(3-Methoxyphenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C27 H30 O7 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

$$\begin{array}{c} \text{Me-S-O} \\ \text{Me-S-O} \\ \text{O} \\ \text{O} \\ \text{O} \\ \text{O} \\ \text{CH}_2-\text{CH}_2 \\ \text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{C$$

PAGE 1-B

`∩ OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 12 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 817642-71-0 REGISTRY
- ED Entered STN: 21 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(2-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2-[[2-(2-Fluorophenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C26 H27 F O6 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

$$\begin{array}{c} O \\ Me-S-O \\ O \\ O \\ O \\ CH_2-CH_2 \\ \end{array} \begin{array}{c} CO_2H \\ F \\ CH_2-CH_2-CH_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 13 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817642-69-6 REGISTRY

ED Entered STN: 21 Jan 2005

CN Benzenepropanoic acid, α -[[2-[4-(dimethylamino)phenyl]ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME) OTHER NAMES:

CN 2-[[2-[4-(Dimethylamino)phenyl]ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid

MF C28 H33 N O6 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

PAGE 1-A

$$\begin{array}{c} \circ \\ \parallel \\ \text{Me-S-O} \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH-S-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__NMe2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 14 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 817209-96-4 REGISTRY
- ED Entered STN: 20 Jan 2005
- CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoic acid (1:1) (9CI) (CA INDEX NAME)

MF C26 H27 O7 S2 . C5 H14 N O

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 840494-28-2 CMF C26 H27 O7 S2

PAGE 1-A

$$\begin{array}{c} \begin{array}{c} \\ \text{Me-s-o} \\ \\ \text{O} \end{array} \\ \begin{array}{c} \text{CO}_2^- \\ \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 62-49-7 CMF C5 H14 N O

 $Me_3+N-CH_2-CH_2-OH$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 15 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-95-3 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, $\alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with tricyclo[3.3.1.13,7]decan-1-amine (1:1) (9CI) (CA INDEX NAME)$

MF C26 H28 O7 S2 . C10 H17 N

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

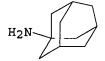
CRN 549494-28-2 CMF C26 H28 O7 S2

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CM 2

CRN 768-94-5 CMF C10 H17 N



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 16 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-93-1 REGISTRY

ED Entered STN: 20 Jan 2005

CN L-Lysine, mono [α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benzenepropanoate] (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . C6 H14 N2 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

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__ OH

CM 2

CRN 56-87-1

CMF C6 H14 N2 O2

Absolute stereochemistry.

$$NH_2$$
 HO_2C
 S
 (CH_2)
 4
 NH_2

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 17 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-92-0 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2 . C4 H11 N O3

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c|c} O & CO_2H \\ \hline \\ O & CH_2-CH_2 \\ \hline \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 77-86-1 CMF C4 H11 N O3

$$\begin{array}{c} & \text{NH}_2 \\ | \\ \text{HO-CH}_2 - \text{C-CH}_2 - \text{OH} \\ | \\ \text{CH}_2 - \text{OH} \end{array}$$

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 18 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-91-9 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with piperazine (1:1) (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2 . C4 H10 N2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

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PAGE 1-B

__ OH

CM 2

CRN 110-85-0 CMF C4 H10 N2

NH

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 19 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817209-90-8 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

MF C26 H28 O7 S2 . C4 H11 N

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

PAGE 1-B

CM 2

CRN 75-64-9 CMF C4 H11 N

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 20 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 817181-58-1 REGISTRY

ED Entered STN: 20 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 21 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 815608-42-5 REGISTRY

ED Entered STN: 18 Jan 2005

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, sodium salt, (α S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 O7 S2 . x Na

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CRN (549494-39-5)

Absolute stereochemistry. Rotation (-).

●x Na

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 22 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 815608-41-4 REGISTRY
- ED Entered STN: 18 Jan 2005
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, potassium salt, (α S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 O7 S2 . x K
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL
- CRN (549494-39-5)

Absolute stereochemistry. Rotation (-).

●x K

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 23 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 549494-39-5 REGISTRY
- ED Entered STN: 17 Jul 2003
- CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 O7 S2
- CI COM
- SR CA
- LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 6 REFERENCES IN FILE CA (1907 TO DATE)
- 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 24 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 549494-32-8 REGISTRY
- ED Entered STN: 17 Jul 2003
- CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H27 Cl O6 S2
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L5 ANSWER 25 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 549494-29-3 REGISTRY
- ED Entered STN: 17 Jul 2003
- CN Benzenepropanoic acid, α -[[2-(4-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)
- MF C26 H27 F O6 S2
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

$$\begin{array}{c} O \\ \parallel \\ \text{Me} \\ -S \\ -O \\ \end{array}$$

$$\begin{array}{c} \text{CO}_2\text{H} \\ -\text{CH}_2 \\$$

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 26 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 549494-28-2 REGISTRY

ED Entered STN: 17 Jul 2003

CN Benzenepropanoic acid, $\alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)$

MF C26 H28 O7 S2

CI COM

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

PAGE 1-A

PAGE 1-B

__ OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 27 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN

RN 549494-27-1 REGISTRY

ED Entered STN: 17 Jul 2003

CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

MF C26 H27 C1 O6 S2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \\ \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2\text{-CH-s-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ C1

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 225.65 572.07

FULL ESTIMATED COST

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FILE 'REGISTRY' ENTERED AT 15:51:34 ON 07 JUN 2007

L1 STRUCTURE UPLOADED

L2 0 S L1 SSS FULL

L3 0 S L1 FULL

FILE 'REGISTRY' ENTERED AT 15:55:27 ON 07 JUN 2007

L4 STRUCTURE UPLOADED

L5 27 S L4 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:57:22 ON 07 JUN 2007

=> s 15 ibib ab hitstr tot
MISSING OPERATOR L5 IBIB
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s 15 L6 7 L5

=> d l6 ibib ab hitstr tot

L6 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:608744 CAPLUS

DOCUMENT NUMBER:

145:83117

TITLE:

Preparation of amine salts of (-)-2-((2-(4-hydroxyphenyl)ethyl)thio)-3-(4-(2-(4-hydroxyphenyl)ethyl)thio)

((methylsulfonyl)oxy) phenoxy)ethyl)phenyl) propanoic acid for treating lipid disorders Snape, Evan William Astrazeneca AB, Swed.; Astrazeneca UK Limited PCT Int. Appl., 24 pp. CODEN: PIXXD2 Patent English FAMILY ACC. NUM. COUNT: KIND DATE APPLICATION NO. DATE ----WO 2005-GB4829 **A**1 20060622 20051214 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM GB 2004-27701 A 20041217 A cinchonidine salt, an (R) - (+) - 1 - (1-naphthyl) ethylamine salt and a (S)-(-)-1-(2-naphthyl)ethylamine salt of the title compound (I) processes for their preparation, their use in treating clin. conditions including lipid disorders (dyslipidemias) whether or not associated with insulin resistance and other manifestations of the metabolic syndrome, and pharmaceutical compns. containing them, are described. 892396-73-5P 892396-76-8P 892396-78-0P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (preparation of amine salts of (-)-2-((2-(4-hydroxyphenyl)ethyl)thio)-3-(4-(2-(4-((methylsulfonyl)oxy) phenoxy)ethyl)phenyl) propanoic acid for treating lipid disorders) 892396-73-5 CAPLUS Cinchonan-9-ol, $(8\alpha, 9R)$ -, mono $[(-)-\alpha-[[2-(4$ hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoate] (salt) (9CI) (CA INDEX NAME)

CM 1

IT

RN

CN

INVENTOR (S):

DOCUMENT TYPE:

SOURCE: ·

LANGUAGE:

PATENT ASSIGNEE(S):

PATENT INFORMATION:

PATENT NO.

WO 2006064232

PRIORITY APPLN. INFO.:

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM

CRN 485-71-2 CMF C19 H22 N2 O Absolute stereochemistry. Rotation (-).

RN 892396-76-8 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (αR) - α -ethyl-1-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

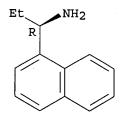
CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 22038-83-1 CMF C13 H15 N

Absolute stereochemistry.



RN 892396-78-0 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with (α S)- α -ethyl-2-naphthalenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-39-5

Absolute stereochemistry. Rotation (-).

CM 2

CRN 254437-90-6 CMF C13 H15 N

Absolute stereochemistry.

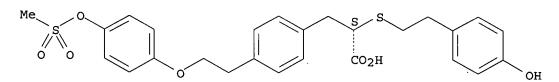
IT 549494-39-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amine salts of (-)-2-((2-(4-hydroxyphenyl)ethyl)thio)-3-(4-(2-(4-((methylsulfonyl)oxy) phenoxy)ethyl)phenyl) propanoic acid for treating lipid disorders)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:608672 CAPLUS

DOCUMENT NUMBER:

145:61508

TITLE:

Chemoenzymic synthesis of 3-phenyl-2arylalkylthiopropionic acid derivatives

INVENTOR(S):

arylalkylthiopropionic acid derivatives Brown, David; Gilday, John Peter; Hopes, Philip

Anthony; Moseley, Jonathan David; Snape, Evan William;

Wells, Andrew

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT	NO.			KIN	D :	DATE			APPLICATION NO. DATE								
	WO 2006		A2 20060622					WO 2	 005-(GB48		20051214						
	WO 2006						2006											
	₩:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KM,	KN,	ΚP,	KR,	
		KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	
		MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	ΡL,	PΤ,	RO,	RU,	SC,	SD,	SE,	
		SG,	SK,	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UZ,	VC,	
	DE			ZA,			~-											
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	
		15,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	МL,	MR,	NE,	SN,	TD,	TG,	BW,	GH,	
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,	
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	RL: BMF	(Bi	oind	ustr:	ial r	nanu	facti	ure)	; BI	OL (1	Biol	ogica	al si	tudv') : PI	REP		
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	(che	moen	zymi	c syı	nthe	sis (of 3	-phei	nyl-:	2-ary	/lal	cyltł	iopi	ropio	onic	acio	3	
	deri	vs.)		-				-	-	•	•	-	1				-	
RN	891182-																	
CN	Benzene	prop	anoi	c ac:	id, 4	1-[2	- [4-	[(met	hyl	sulfo	onyl	oxy]	pher	noxy	ethy	/1]-c	χ –	
	[(2-phe	nyle	thyl)thic	o] -,	(as) - (9CI)	(C	A INI	DEX 1	NAMĒ)	ı	•	-	-		

Absolute stereochemistry.

IT 549494-39-5P

RL: BPN (Biosynthetic preparation); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 817181-58-1P

RL: BYP (Byproduct); PREP (Preparation)
 (chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid
 derivs.)

RN 817181-58-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (αR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 891182-81-3P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN -891182-81-3 CAPLUS

CN Benzenepropanoic acid, $\alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)$

CM 1

CRN 549494-39-5 CMF C26 H28 O7 S2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 75-64-9 CMF C4 H11 N

IT 549494-28-2

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid derivs.)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} O \\ He - S - O \\ CH_2 - CH_2 \\ \end{array}$$

PAGE 1-B

__ OH

817209-90-8P IT

RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(chemoenzymic synthesis of 3-phenyl-2-arylalkylthiopropionic acid

derivs.)

817209-90-8 CAPLUS RN

Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-CN[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-S-O} \\ \circ \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \\ \begin{array}{c} \text{CO}_2\text{H} \\ \circ \\ \text{CH}_2\text{-CH-S-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 75-64-9 CMF C4 H11 N

 NH_2 H₃C -CH3 CH₃

ACCESSION NUMBER: 2004:1154663 CAPLUS DOCUMENT NUMBER: 142:93390 TITLE: Process for the preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative, useful as selective PPAR α modulator INVENTOR(S): Andersson, Kjell; Lindstedt-Astermark, Eva-Lotte; Sorensen, Henrik PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.; Astrazeneca Uk Limited SOURCE: PCT Int. Appl., 17 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. -----------WO 2004113285 A1 20041229 WO 2004-GB2599 20040616 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR; HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2004249487 Α1 20041229 AU 2004-249487 20040616 CA 2529252 Α1 20041229 CA 2004-2529252 20040616 EP 1638929 EP 2004-736920 A1 20060329 20040616 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR BR 2004011450 Α 20060718 BR 2004-11450 20040616 CN 1835918 Α 20060920 CN 2004-80023145 20040616 JP 2006527751 Т 20061207 JP 2006-516435 20040616 NO 2005005883 Α 20060109 NO 2005-5883 20051212 US 2006167309 A1 20060727 US 2005-561161 20051216 PRIORITY APPLN. INFO.: GB 2003-14260 A 20030619 WO 2004-GB2599 W 20040616 OTHER SOURCE(S): CASREACT 142:93390; MARPAT 142:93390 The invention provides a process for preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative of formula I, useful as selective PPAR α modulator (no biol. data). The racemic title compound I was prepared via thiolation of 2-chloropropanoate derivative II by 2-[4-(benzyloxy)phenyl]ethanethiol, debenzylation, and hydrolysis. Resolution of I gave (-)-I and (+)-I. (+)-Enantiomer was used as a starting material for racemization reaction. IT 549494-39-5P RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation) (process for the preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative useful as selective PPAR α modulator) 549494-39-5 CAPLUS RNCNBenzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (\alphaS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-28-2P 817181-58-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for the preparation of racemic [(hydroxyphenyl)ethylthio]propanoic acid derivative useful as selective PPARa modulator)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \end{array}$$

PAGE 1-B

__ OH

RN 817181-58-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

5

ACCESSION NUMBER:

2004:1154662 CAPLUS

DOCUMENT NUMBER:

142:86664

TITLE:

SOURCE:

Potassium or sodium salt of $(-)-2-\{[2-(4-$

hydroxyphenyl) ethyl] thio $\}$ -3-[4-(2- $\{4$ -

[(methylsulfonyl)oxy]phenoxy}ethyl)phenyl]propanoic

acid and their use in medicine

INVENTOR(S):

Ahlqvist, Matti; Bohlin, Martin Hans

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
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     WO 2004113284
                         A1
                                 20041229
                                             WO 2004-GB2595
                                                                     20040616
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE,
             SN, TD, TG
     AU 2004249485
                                 20041229
                          A1
                                             AU 2004-249485
                                                                     20040616
     CA 2529251
                          A1
                                 20041229
                                             CA 2004-2529251
                                                                     20040616
     EP 1641749
                          Α1
                                 20060405
                                             EP 2004-742954
                                                                     20040616
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
     BR 2004011515
                          Α
                                 20060801
                                             BR 2004-11515
                                                                     20040616
     CN 1835920
                          Α
                                 20060920
                                             CN 2004-80023294
                                                                     20040616
     JP 2006527750
                          Т
                                 20061207
                                             JP 2006-516434
                                                                     20040616
     NO 2005005927
                          Α
                                 20060127
                                             NO 2005-5927
                                                                     20051213
     US 2007099997
                                             US 2005-561170
                          A1
                                 20070503
                                                                     20051216
PRIORITY APPLN. INFO.:
                                             GB 2003-14131
                                                                  Α
                                                                     20030618
                                             WO 2004-GB2595
                                                                  W
                                                                     20040616
AB
     A potassium salt or a sodium salt of (-)-2-\{[2-(4-
     hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl)ph
     enyl]propanoic acid, processes for their preparation, their use in treating
     clin. conditions including lipid disorders (dyslipidemias) whether or not
     associated with insulin resistance and other manifestations of the metabolic
     syndrome, and pharmaceutical compns. containing them.
ΙT
     815608-41-4P 815608-42-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of potassium or sodium salt of (-)-2-{[2-(4-
        hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl
        )phenyl]propanoic acid for therapeutic use)
RN
     815608-41-4 CAPLUS
     Benzenepropanoic acid, \alpha-[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-
CN
     [(methylsulfonyl)oxy]phenoxy]ethyl]-, potassium salt, (\alpha S)- (9CI)
```

Absolute stereochemistry. Rotation (-).

●x K

RN 815608-42-5 CAPLUS

(CA INDEX NAME)

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, sodium salt, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

●x Na

IT 549494-39-5P

RL: PUR (Purification or recovery); PREP (Preparation)

(preparation of potassium or sodium salt of $(-)-2-\{[2-(4-$

hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl

)phenyl]propanoic acid for therapeutic use)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-28-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of potassium or sodium salt of (-)-2-{[2-(4-

hydroxyphenyl)ethyl]thio}-3-[4-(2-{4-[(methylsulfonyl)oxy]phenoxy}ethyl

)phenyl]propanoic acid for therapeutic use)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me}-\text{S}-\text{O} \\ \circ \\ \circ \\ \text{O} \\ \end{array}$$

PAGE 1-B

__ OH

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:1154661 CAPLUS

DOCUMENT NUMBER:

142:93515

TITLE:

A preparation of amine salts of

[(phenoxyethyl)phenyl]propanoic acid derivative,

useful for the treatment of lipid disorders

INVENTOR (S):

Ahlqvist, Matti; Dahlstrom, Mikael Ulf Johan; Ohlsson,

Bengt; Storey, Richard Anthony; Taylor, Nigel Philip;

Woods, Rebecca

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 43 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

TZ T NTD

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION: DAMENIO NO

	PA	CENT :	NO.			KIND DATE													
	WO	2004	1132	83						WO 2004-GB2576									
												BG,							
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,	
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
			NO,	ΝZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
			ТJ,	TM,	TN,	TR,	TT,	TZ,	UΑ,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
												BE,							
			EE,	ES,	FI,	FR,	GB,	GR;	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	
			SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	
			-	TD,															
	ΑU	CA 2529544 EP 1638930				A1 20041229				AU 2004-249483						20040616			
									CA 2004-2529544										
	ĒΡ										EP 2004-736922								
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	ΝL,	SE,	MC,	PT,	
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR
	BR 2004011580 CN 1835919 JP 2006527749					Α		2006	8080]	BR 2004-11580					20040616			
						A 20060920				(JP 2006-516428					20040616			
									t										
		2005						2006	0224]	NO 2	005-	6006			20	00512	216	
		2007				A1		2007	0503	1	US 2	005-	56122	22		20	00512	219	
RIO	RIT	APP	LN.	INFO	. :					(GB 2	003-	1413	0	1	A 20	00306	518	
										1	WO 2	004-	GB25	76	V	V 20	0406	516	
۱B	The	e inv	entid	on re	-la+.	e to	n a	nren	arat.	ion /	_ +	024	h,,+,-	1 ~~		. 7	2		·

The invention relates to a preparation of tert-butylamine salt, piperazine AB salt, choline salt, tris(hydroxymethyl)methylamine salt, lysine salt, or adamantylamine salt of [(phenoxyethyl)phenyl]propanoic acid derivative of formula (-)-I, useful in the treatment of lipid disorders (no biol. data). Tert-Butylamine salt of (-)-I was prepared from (-)-I and tert-butylamine with a yield of 68% (example 1).

IT 817209-90-8P 817209-91-9P 817209-92-0P 817209-93-1P

> RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative

useful for the treatment of lipid disorders)

ВM 817209-90-8 CAPLUS

Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-CN [(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-methyl-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-S-O} \\ \circ \\ \circ \\ \text{O} \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 75-64-9 CMF C4 H11 N

RN 817209-91-9 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with piperazine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c} O \\ Me-s-O \\ O \\ O \\ O \\ O \\ CH_2-CH_2 \\ \end{array} \begin{array}{c} CO_2H \\ CH_2-CH_2-CH_2 \\ \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 110-85-0 CMF C4 H10 N2

RN 817209-92-0 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

PAGE 1-B

__ OH

CM 2

CRN 77-86-1 CMF C4 H11 N O3

$$\begin{array}{c} ^{\rm NH_2} \\ _{\rm HO-CH_2-C-CH_2-OH} \\ _{\rm CH_2-OH} \end{array}$$

RN 817209-93-1 CAPLUS

CN L-Lysine, mono [α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benzenepropanoate] (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

__ OH

CM 2

CRN 56-87-1 CMF C6 H14 N2 O2

Absolute stereochemistry.

IT 817209-95-3P 817209-96-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

 $(\mbox{preparation of a mine salts of [(phenoxyethyl)phenyl]propanoic acid derivative}$

useful for the treatment of lipid disorders)

RN 817209-95-3 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, compd. with tricyclo[3.3.1.13,7]decan-1-amine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 549494-28-2 CMF C26 H28 O7 S2

PAGE 1-A

$$\begin{array}{c|c} O & CO_2H \\ \hline \\ O & CH_2-CH_2 \\ \hline \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 768-94-5 CMF C10 H17 N

RN 817209-96-4 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, salt with α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]benze nepropanoic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 840494-28-2 CMF C26 H27 O7 S2

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \end{array}$$

PAGE 1-B

__ OH

CM 2

CRN 62-49-7 CMF C5 H14 N O

 $Me_3+N-CH_2-CH_2-OH$

IT 549494-39-5P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative

useful for the treatment of lipid disorders)

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-28-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of amine salts of [(phenoxyethyl)phenyl]propanoic acid derivative

useful for the treatment of lipid disorders)

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

3

ACCESSION NUMBER:

2004:1154660 CAPLUS

DOCUMENT NUMBER:

142:93534

TITLE:

Substituted 3-phenylpropionic acid derivatives with

PPAR α and PPAR δ modulatory activities,

useful as therapeutic agents for treatment of

dyslipidemia, and their preparation, pharmaceutical

compositions, and methods of use

INVENTOR(S):

Lindstedt-Alstermark, Eva-Lotte; Boije, Anna Maria

Persdotter; Holm, Patrik

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 52 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIN	D :	DATE		APPLICATION NO.									
WO 2004113282					A1	-	2004	 1229						20040616				
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR.	BW.	BY.	BZ.	CA.	CH.	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG.	ES.	FI.	GB.	GD.	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE.	KG.	KP.	KR.	KZ.	LC.	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN.	MW.	MX.	MZ.	NA.	NT.	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc.	SD.	SE.	SG.	SK.	SI.	SY,	
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪĠ.	us.	UZ.	VC.	VN.	YU.	7A.	2M	2W	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL.	SZ.	TZ.	UG.	ZM.	ZW .	ΔM	
		ΑZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG.	CH.	CY.	CZ.	DE.	DK	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT.	LU.	MC.	NL.	PL.	PT.	RO.	SE,	
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM.	GA.	GN.	GO.	GW.	MT.	MR	NE	
		SN,	TD,	TG		-	•		•	•	,	,	- = /	J.,	,	,	,	
AU 2004249474				A1	:	2004	1229	AU 2004-249474						21	0040	040616 CA, CH, GB, GD, KZ, LC, NA, NI, SL, SY, ZM, ZW ZW, AM, DE, DK, RO, SE, MR, NE,		
CA 2529297				A1				CA 2004-2529297										
EΡ	1638927						EP 2004-736926											
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR.	IT.	LI.	LU.	NT.	SE.	MC'	DT.	
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ.	EE.	HU.	PI.	SK.	нр

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BR 2004011536
                         Α
                                20060801
                                           BR 2004-11536
                                                                   20040616
    CN 1835917
                         A
                               20060920
                                           CN 2004-80023273
                                                                   20040616
    JP 2006527747
                         T
                                20061207
                                           JP 2006-516423
                                                                   20040616
    NO 2005006005
                         Α
                                20060224
                                           NO 2005-6005
                                                                   20051216
    US 2006199857
                         A1
                                20060907
                                           US 2005-561126
                                                                   20051216
PRIORITY APPLN. INFO.:
                                           GB 2003-14075
                                                                   20030618
                                           WO 2004-GB2554
                                                                W 20040616
```

OTHER SOURCE(S): MARPAT 142:93534

RN

CN

Substituted 3-phenylpropionic acid derivs. I are disclosed [R = H, OH or NH or their derivs.; R1 = alk(en/yn)yl, aryl, cyano, OH or SH or CO2H or their derivs.; R2 = H, alkyl, aryl, alkylaryl; R3, R4 = (independently) H, alkyl, aryl, alkylaryl; or R2R4 = pi bond; n = 1-6; m = 0 or 1; D's = H or wide variety of substituents; T = O, S, or N(X) with some restrictions; X = alkyl or alkylaryl; with 2 complex provisos]. Also disclosed are (1) processes for preparing I, (2) their utility in treating clin. conditions including lipid disorders (dyslipidemias), whether or not associated with insulin resistance and other manifestations of the metabolic syndrome, (3) methods for their therapeutic use, and (4) pharmaceutical compns. containing them. I were tested in the assays described in WO 03/051821 (no data). I show superior potency in vitro, higher affinity, and/or higher in vivo efficacy. I also have a better selectivity profile, which is expected to improve in vivo safety. In addition, I may have improved DMPK (drug metabolism and pharmacokinetic) properties, for example improved metabolic stability in vitro or bioavailability. The compds. also have an improved solubility and/or a promising toxicol. profile. I may be combined with other therapeutic agents that are useful in the treatment of disorders associated with the development and progress of atherosclerosis such as hypertension, hyperlipidemias, dyslipidemias, diabetes and obesity. Twelve examples were prepared and/or claimed. For instance, compound II was prepared by: (1) thioetherification of 4-(PhCH2O)C6H4CH2CH2SH with ClCH(CO2Me)CH2C6H4(CH2CH2OH)-4 (40%); (2) Mitsunobu etherification of the product alc. with 4-benzoylphenol (83%); (3) debenzylation (78%); and (4) saponification of the ester with LiOH (49%). The EC50 of II for human PPARlphawas $0.78 \mu M$.

IT 817642-69-6P, 2-[[2-[4-(Dimethylamino)phenyl]ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-71-0P, 2-[[2-(2-Fluorophenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-72-1P, 2-[[2-(3-Methoxyphenyl)ethyl]thio]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-73-2P, 2-[[2-(4-Hydroxyphenyl)ethyl]sulfinyl]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-76-5P, 2-[[2-(4-Hydroxyphenyl)ethyl]sulfonyl]-3-[4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]phenyl]propanoic acid 817642-78-7P, 3-[4-[2-[2-Benzyl-4-[(methanesulfonyl)oxy]phenoxy]et hyl]phenyl]-2-[[2-(4-hydroxyphenyl)ethyl]sulfanyl]propionic acid 817642-79-8P, 2-[[2-(4-Tert-Butoxyphenyl)ethyl]sulfanyl]-3-[4-[2-[4-[(methanesulfonyl)oxy]phenoxy]ethyl]phenyl]propionic acid RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of substituted phenylpropionic acid derivs. as PPAR α and PPAR δ modulators for treatment of dyslipidemia) 817642-69-6 CAPLUS

Benzenepropanoic acid, α -[[2-[4-(dimethylamino)phenyl]ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

-NMe₂

RN 817642-71-0 CAPLUS

CN Benzenepropanoic acid, α -[[2-(2-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

RN 817642-72-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(3-methoxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

Me—S=0
$$CH_2$$
 CH_2 CH_2

PAGE 1-B

[→] OMe

RN 817642-73-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfinyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c|c} & & & & & \\ & & & & \\ \text{Me}-\text{S}-\text{O} & & & \\ & & & \\ & & & \\ \text{O} & & & \\ & & & \\ & & & \\ \end{array}$$

__ OH

RN 817642-76-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]sulfonyl]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

RN 817642-78-7 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]-2-(phenylmethyl)phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} O \\ \parallel \\ Ne-S-O \\ \parallel \\ O \\ CH_2-CH_2 \end{array} \begin{array}{c} CO_2H \\ CH_2-CH_2-CH_2 \end{array}$$

PAGE 1-B

__ OH

RN 817642-79-8 CAPLUS

CN Benzenepropanoic acid, α -[[2-[4-(1,1-dimethylethoxy)phenyl]ethyl]thi o]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2003:491173 CAPLUS

DOCUMENT NUMBER:

139:69050

TITLE:

Preparation of 3-phenyl-2-arylalkylthiopropionic acid

derivatives as selective agonists of PPAR- α

INVENTOR(S):

Alstermark Lindstedt, Eva-Lotte; Persdotter Boije,

Anna Maria; Holm, Patrik

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 47 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.					KIND		DATE		APPLICATION NO.				DATE			
	2003051826								WO 2002-GB5743								
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB	, BG,	BR,	BY,	BZ,	CA,	CH.	CN.
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC	, EE,	ES,	FI,	GB,	GD.	GE.	GH.
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE	, KG,	KP,	KR,	KZ,	LC,	LK,	LR.
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN	, MW,	MX,	MZ,	NO,	NZ,	OM.	PH.
		PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK	, SL,	TJ,	TM,	TN,	TR.	TT.	TZ.
		UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM	, ZW						
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ	, TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	ΚZ,	MD,	RU,	TJ,	TM,	ΑT,	BE,	BG	, CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	· NL	, PT,	SE,	SI,	SK,	TR,	BF,	ВJ,
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PRIORITY APPLN. INFO.:									2001-					0011			
											2003-						
OTHER CO	מטמוור	/O\ .								WO	2002-	GB57	43	1	W 2	0021	218

OTHER SOURCE(S): MARPAT 139:69050

AB 4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)CH2CH2C6H4R-4 [I, R = Cl, F, OH] and optical isomers and racemates thereof were prepared for use in treating clin. conditions including lipid disorders (dyslipidemias) whether or not associated with insulin resistance. I have EC50 \leq 5 μmol/L for PPAR-α and the ratio EC50(PPAR-γ):EC50(PPAR-α) > 25:1. Thus, I [R = Cl] was prepared from 4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)Cl

and 4-ClC6H4CH2CH2SH.

IT 549494-32-8P 549494-39-5P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α)

RN 549494-32-8 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

RN 549494-39-5 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 549494-27-1P 549494-28-2P 549494-29-3P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs. as selective agonists of PPAR- α)

RN 549494-27-1 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-chlorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-s-o} \\ \circ \\ \circ \\ \text{O} \end{array}$$

PAGE 1-B

__ c1

RN 549494-28-2 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-hydroxyphenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-s-O \\ O \\ O \\ O \\ O-CH_2-CH_2 \\ \end{array} \\ \begin{array}{c} CO_2H \\ CH_2-CH-s-CH_2-CH_2 \\ \end{array}$$

PAGE 1-B

__ OH

RN 549494-29-3 CAPLUS

CN Benzenepropanoic acid, α -[[2-(4-fluorophenyl)ethyl]thio]-4-[2-[4-[(methylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \circ \\ \text{Me-S-O} \\ \circ \\ \circ \\ \circ \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c} \text{CO}_2\text{H} \\ \circ \\ \text{CH}_2\text{-CH-S-CH}_2\text{-CH}_2 \\ \end{array}$$

PAGE 1-B

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ACCESSION NUMBER:

2003:491173 CAPLUS

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Entered STN: 27 Jun 2003

TITLE:

Preparation of 3-phenyl-2-arylalkylthiopropionic acid

derivatives as selective agonists of PPAR- α

INVENTOR(S):

Alstermark Lindstedt, Eva-Lotte; Persdotter Boije, .

Anna Maria; Holm, Patrik

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 47 pp. CODEN: PIXXD2

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LANGUAGE:

English

INT. PATENT CLASSIF.:

MAIN:

C07C323-56

SECONDARY:

A61K031-192

CLASSIFICATION:

25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

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                          MARPAT 139:69050
OTHER SOURCE(S):
ABSTRACT:
4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)CH2CH2C6H4R-4 [I, R = Cl, F, OH] and
optical isomers and racemates thereof were prepared for use in treating clin.
conditions including lipid disorders (dyslipidemias) whether or not associated
with insulin resistance. I have EC50 \leq 5 \mu mol/L for PPAR-\alpha and
the ratio EC50(PPAR-\gamma):EC50(PPAR-\alpha) > 25:1. Thus, I [R = Cl] was
prepared from 4-(4-MeSO3C6H4OCH2CH2)C6H4CH2CH(CO2H)Cl and 4-C1C6H4CH2CH2SH.
SUPPL. TERM:
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aralkylthiophenylpropanoic acid prepn peroxisome proliferator activated receptor modulator

INDEX TERM: Dyslipidemia

ROLE: BSU (Biological study, unclassified); BIOL (Biological

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study)
                       (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs.
                       as selective agonists of PPAR-\alpha)
INDEX TERM:
                   Peroxisome proliferator-activated receptors
                   ROLE: BSU (Biological study, unclassified); BIOL (Biological
                   study)
                       (\alpha; preparation of 3-phenyl-2-arylalkylthiopropionic
                       acid derivs. as selective agonists of PPAR-\alpha)
INDEX TERM:
                   549494-32-8P
                                   549494-39-5P
                   ROLE: PUR (Purification or recovery); SPN (Synthetic
                   preparation); THU (Therapeutic use); BIOL (Biological
                   study); PREP (Preparation); USES (Uses)
                       (preparation of 3-phenyl-2-arylalkylthiopropionic acid derivs.
                       as selective agonists of PPAR-\alpha)
INDEX TERM:
                   96-33-3, Methyl acrylate
                                              103-16-2, 4-Benzyloxyphenol
                   104-10-9, 2-(4-Aminophenyl)ethanol 332-43-4,
                   1-(2-Chloroethyl)-4-fluorobenzene
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                                      32327-70-1, 1-Chloro-4-(2-
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                                          549494-36-2
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REFERENCE COUNT:
                   2
                          THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
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REFERENCE(S):
                    (1) Astra; WO 9962871 A 1999 CAPLUS
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(2) Astra; WO 9962872 A 1999 CAPLUS